Dynamic virial theorem at nonequilibrium and applications

Shi-Guo Peng *

State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Innovation Academy for Precision Measurement Science and Technology, Chinese Academy of Sciences, Wuhan 430071, China

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We show that a variety of nonequilibrium dynamics of interacting many-body systems are universally characterized by an elegant relation, which we call the dynamic virial theorem. The out-of-equilibrium dynamics of quantum correlations is entirely governed by Tan' s contact. It gives rise to a series of observable consequences and is closely related to experiments with ultracold atoms. In particular, we show that the dynamic virial theorem provides an experimentally accessible verification of the maximum energy growth theorem [R. Qi *et al.*, Phys. Rev. Lett. **126**, 240401 (2021)], which is encoded in the evolution of the atomic cloud size during expansion. In addition, the dynamic virial theorem leads to a simple thermodynamic relation of strongly interacting quantum gases in the framework of two-fluid hydrodynamic theory, which holds in a wide range of temperature. This thermodynamic relation is a type of out-of-equilibrium analog of Tan's pressure relation at equilibrium. Our results provide a fundamental understanding of the generic behaviors of interacting many-body systems at nonequilibrium and are readily examined in experiments with ultracold atoms.

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I. INTRODUCTION

The investigation of nonequilibrium dynamics of strongly interacting many-body systems is of fundamental importance and remains an open challenge in modern physics, while it is broadly relevant to many phenomena in the universe, ranging from the evolution of neutron stars and the procedure of chemical reactions, to complex living systems in biology. The discovery of universal features in quantum systems at nonequilibrium, irrelevant to the microscopic detail of the studied objects, is a longstanding challenge to date and attracts a great deal of attention in both theory and experiment. Ultracold atoms, as clean, controllable, and versatile quantum systems, provide an unprecedented platform for the exploration of a wide variety of phenomena in many-body physics, ranging from thermodynamic equilibrium to out-of-equilibrium dynamics [1–6]. Remarkably, ultracold atomic systems have unique advantages for the study of nonequilibrium dynamics within experimentally resolved intrinsic timescales (typically milliseconds), holding promising opportunities to test the universality of many-body dynamics far from equilibrium [7–13].

A set of universal relations in cold atoms, connected by a simple contact parameter, has been discovered [14–16]. These relations simply follow from the short-range correlation of two-body physics and provide a remarkable understanding of the profound properties of interacting many-body systems. To date, an impressive amount of experimental and theoretical effort has been devoted to confirm the universal relations and explore their important consequences [17–24]. While most of them are focused on the properties of many-body systems at equilibrium, the universal relations at nonequilibrium are rarely studied and still remain elusive.

In this work, it is found that a variety of dynamic processes of many-body systems driven away from equilibrium by either the time-dependent external potential or time-dependent interactions are elegantly governed by the dynamic virial theorem. These are the favorite ways to study the out-of-equilibrium dynamics in experiments of cold atoms, such as the expansion dynamics [25,26] and the interaction quench [7–10,13]. The dynamic virial theorem reveals a deep insight into the precise energy conversion relation, i.e.,

$$E(t) - 2E_{\rm ho}(t) = \frac{1}{4}\frac{d^2 I(t)}{dt^2} - \frac{\hbar^2 \mathcal{C}(t)}{8\pi m a(t)}, \tag{1}$$

which imposes an intrinsic constraint on the energy dynamics. Here, m is the atomic mass, $\hbar$ is Planck's constant, and $a(t)$ is the scattering length generally varying in time. $E_{\rm ho}(t)$ is the energy corresponding to the external harmonic potential, $I(t) \equiv \langle mr^2 \rangle$ is the moment of inertia of the systems, and $\mathcal{C}(t)$ is Tan's contact [14–16]. In the classical (or high-temperature) limit, the kinetic energy dominates the internal energy. The dynamic virial theorem immediately implies an interesting nondamping monopole oscillation with twice the trapping frequency in a perfectly spherical trap, and systems never reach thermal equilibrium. This long-predicted phenomenon by Boltzmann's equation has recently been observed by JILA's group in a thermal Bose gas [27]. In the quantum (or low-temperature) limit, the interaction between particles comes into play and shifts the frequency of the monopole oscillation [28–31]. We find that the dynamics of the quantum correlations is entirely governed by Tan's contact. In the unitarity limit with divergent scattering length, the systems display scale invariance. The dynamic virial theorem requires

*pengshiguo@wipm.ac.cn

a unitary gas to exactly follow the same dynamics of an ideal gas [25,26,32]. At equilibrium, the dynamic virial theorem simply recovers that of [16] at finite interaction strength, and further reduces to the well-known equilibrium result of $E = 2E_{\rm ho}$ for unitary and ideal gases [33].

The applications of the dynamic virial theorem are demonstrated in several typical dynamic processes. The observable consequences in experiments of ultracold atoms are discussed. There are two typical ways to study the nonequilibrium dynamics in experiments with cold atoms, i.e., in a time-dependent trap and with a time-dependent interaction. For the former, we show that the release energy of cold atoms during free expansion is directly given by the dynamic virial theorem. The frequencies of monopole oscillations are simply derived according to the dynamic virial theorem. In addition, the dynamic virial theorem simply characterizes the intriguing Efimovian expansion of scale-invariant quantum gases in a time-dependent harmonic trap [26]. For the latter, a fundamental issue has theoretically been addressed recently as to how fast the energy could be pumped into a noninteracting system by increasing interactions [34]. Counterintuitively, it is not true that the faster the interaction increases, the larger the rate of energy gain becomes. Instead, there exists an upper limit of the initial energy growth rate, which could be reached only when the scattering length increases with time t as $\sim\sqrt{t}$, known as the maximum energy growth theorem. However, the direct measurement of the energy dynamics in experiments is difficult. We show that the dynamic virial theorem provides an experimentally accessible way to verify the maximum energy growth theorem according to the expansion behavior of the atomic cloud size. Remarkably, a simple dynamic thermodynamic relation is derived using the dynamic virial theorem in the framework of the two-fluid hydrodynamic theory for interacting quantum gases. This thermodynamic relation is a type of out-of-equilibrium analog of Tan's pressure relation at equilibrium [16] and holds in a wide range of temperatures.

The rest of the paper is arranged as follows. In the next section, we present the brief proof of the dynamic virial theorem for interacting many-body systems. Afterwards, the dynamic virial theorem is applied to study the out-of-equilibrium dynamics for cold atoms in time-dependent harmonic traps, i.e., free expansion (Sec. III), Efimovian expansion (Sec. IV), and monopole oscillation (Sec. V). We show, in Sec. VI, that the dynamic virial theorem provides an experimentally accessible verification of the maximum energy growth theorem by increasing interatomic interactions, which is encoded in the evolution of the atomic cloud size during expansion. An out-of-equilibrium thermodynamic relations is obtained by using the dynamic virial theorem in the framework of the two-fluid hydrodynamic theory in Sec. VII. Finally, the remarks and conclusions are summarized in Sec. VIII.

II. DYNAMIC VIRIAL THEOREM

To prove the dynamic virial theorem (1), let us consider a system consisting of N atoms (either bosons or fermions) in a harmonic trap. The Hamiltonian of the system takes the form of

$$\hat{H} = \hat{H}_0 + \hat{V}_{\rm int}, \tag{2}$$

in which

$$\hat{H}_0 = \sum_{j=1}^{N} \left[\mathbf{p}_j^2/2m + \hat{V}_{\rm ho}(\mathbf{r}_j; t)\right] \tag{3}$$

is the single-particle Hamiltonian, and

$$\hat{V}_{\rm int} = \sum_{ij} \hat{U}[\mathbf{r}_{ij}; a(t)] \tag{4}$$

is the interatomic interactions with $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$. Here, we consider the most general case in which the harmonic potential $\hat{V}_{\rm ho}$ and interatomic interactions both vary in time, i.e., with the time-dependent trapping frequency $\omega(t)$ and s-wave scattering length $a(t)$. The evolution of the moment of inertia $I(t) = \langle\sum_j mr_j^2\rangle \equiv \langle mr^2\rangle$ is governed by the Heisenberg equation, i.e.,

$$\frac{dI}{dt} = \frac{1}{i\hbar}[I, \hat{H}], \tag{5}$$

which simply yields $\dot{I} \equiv dI/dt = 2\langle\hat{D}\rangle$, and $\hat{D} = \sum_{j=1}^{N}(\mathbf{r}_j \cdot \mathbf{p}_j + \mathbf{p}_j \cdot \mathbf{r}_j)/2$ is the generator of scale transformation named the dilatation operator [32,35,36]. By further taking the second-order derivative with respect to time, i.e., $\ddot{I} = 2\langle[\hat{D}, \hat{H}]\rangle/i\hbar$, we obtain

$$\frac{d^2I}{dt^2} = 4\langle\hat{H}\rangle - 8\langle\hat{V}_{\rm ho}\rangle - 4\langle\hat{V}_{\rm int}\rangle + \frac{2}{i\hbar}\langle[\hat{D}, \hat{V}_{\rm int}]\rangle. \tag{6}$$

To proceed, we notice that the two-body interaction $\hat{U}(\mathbf{r}_{ij}; a)$, under the scale transformation, has the property of $e^{-i\epsilon\hat{D}/\hbar}\hat{U}(\mathbf{r}_{ij}; a)e^{i\epsilon\hat{D}/\hbar} = e^{2\epsilon}\hat{U}(\mathbf{r}_{ij}; e^{\epsilon}a)$ for infinitesimal ϵ. Expanding both sides of this equation up to the first-order term of ϵ, we obtain the commutation relation of $[\hat{D}, \hat{U}]$, which in turn gives

$$\frac{1}{i\hbar}\langle[\hat{D}, \hat{V}_{\rm int}]\rangle = 2\langle\hat{V}_{\rm int}\rangle + a\left\langle\frac{\partial\hat{V}_{\rm int}}{\partial a}\right\rangle. \tag{7}$$

Inserting Eq. (7) into Eq. (6) and combining with the Hellmann-Feynman theorem and Tan's relation [15], i.e.,

$$\left\langle\frac{\partial\hat{V}_{\rm int}}{\partial a}\right\rangle = \frac{\partial E}{\partial a} = \frac{\hbar^2\mathcal{C}}{4\pi ma^2}, \tag{8}$$

we finally arrive at Eq. (1) with $E(t) = \langle\hat{H}\rangle$ and $E_{\rm ho}(t) = \langle\hat{V}_{\rm ho}\rangle$. The similar formulism has been obtained in discussing the breathing mode of two-dimensional Fermi gases and the corresponding scale-invariant dynamics, such as the quantum anomaly [37,38]. Here, we emphasize that Eq. (1), as a fundamental analogous relation of virial theorem at equilibrium [33], characterizes a broad variety of nonequilibrium dynamics of interacting quantum gases. It provides a deep insight into generic out-of-equilibrium characters, which we are going to demonstrate as in the following.

III. FREE EXPANSION OF QUANTUM GASES

Free expansion, simply releasing atoms from the trap, provides crucial information on both the equilibrium and dynamic properties of ultracold atomic gases. It is widely used in experiments of cold atoms, such as the time of flight. One of the direct applications of dynamic virial theorem is

to calculate the release energy, i.e., $E_{\rm rel} \equiv E(t)$. Since the release energy is well understood in weakly interacting and unitary gases, it is inversely convenient to verify the validity of the dynamic virial theorem. To this end, the knowledge of evolution of Tan's contact as well as that of the moment of inertia is required. As an example, let us consider free expansion of a two-component Fermi gas, initially prepared at equilibrium in the trap. We evaluate the evolution of Tan's contact and moment of inertia of the system in the framework of hydrodynamic theory [39,40]. To solve the hydrodynamic equations, we adopt the scaling form of the time-dependent density profile, i.e., $n(\mathbf{r},t) = n_0(\mathbf{r}/b)/b^3(t)$, where $n_0(\mathbf{r})$ is the equilibrium density profile initially in the trap. The time dependence of $n(\mathbf{r},t)$ is entirely determined by the scaling factor $b(t)$. The atomic cloud size $\langle r^2\rangle(t)$ during expansion is related to the initial size $\langle r^2\rangle_0$ by the scaling factor $b(t)$ as $\langle r^2\rangle(t) = b^2(t)\langle r^2\rangle_0$, which in turn gives

$$\ddot{I}(t) = \frac{4}{\omega_0}[\dot{b}^2(t) + b(t)\ddot{b}(t)]E_{\rm ho}^{(0)}, \tag{9}$$

where $E_{\rm ho}^{(0)}$ is the initial potential energy and ω_0 is the initial trapping frequency.

In the weakly interacting Bardeen-Cooper-Schrieffer (BCS) limit with small negative scattering length, the scaling factor $b(t)$ satisfies [39,40]

$$\ddot{b}(t) - \frac{\omega_0^2}{b^3(t)} + \frac{3}{2}\chi(g)\omega_0^2\left[\frac{1}{b^3(t)} - \frac{1}{b^4(t)}\right] = 0, \tag{10}$$

where $\chi(g) = E_{\rm int}^{(0)}/E_{\rm ho}^{(0)}$ is the ratio of interaction energy $E_{\rm int}^{(0)}$ to potential energy $E_{\rm ho}^{(0)}$ initially in the trap, and $g = 4\pi\hbar^2 a/m$ is the interaction strength between atoms. The contact $\mathcal{C}(t)$ during expansion may be evaluated according to the local density approximation (LDA) by making the adiabatic ansatz [41], i.e., $\mathcal{C}(t) = \int d\mathbf{r}\mathcal{I}(\mathbf{r},t)$, with local contact density $\mathcal{I}(\mathbf{r},t) \approx 4\pi^2 n^2(\mathbf{r},t)a^2$ [15], which in turn gives $\mathcal{C}(t) = 4\pi maE_{\rm int}^{(0)}/\hbar^2 b^3$. With all these results in hand, we easily obtain the release energy according to the dynamic virial theorem, i.e.,

$$E_{\rm rel} = E_{\rm ho}^{(0)}\left\{\frac{1}{\omega_0^2}[\dot{b}^2(t) + b(t)\ddot{b}(t)] - \frac{\chi(g)}{2b^3(t)}\right\}. \tag{11}$$

From Eq. (10), we find [42]

$$\frac{1}{\omega_0^2}[\dot{b}^2(t) + b(t)\ddot{b}(t)] = 1 - \frac{1}{2}\chi(g)\left[1 - \frac{1}{b^3(t)}\right]. \tag{12}$$

Then the release energy reads

$$E_{\rm rel} = \left[1 - \tfrac{1}{2}\chi(g)\right]E_{\rm ho}^{(0)} \tag{13}$$

in the weakly interacting limit, and further reduces to the well-known result $E_{\rm rel} = E_{\rm ho}^{(0)}$ in the BCS limit [2].

In the Bose-Einstein-Condensation (BEC) limit with small positive scattering length, the scaling factor satisfies [40]

$$\ddot{b}(t) - \frac{\omega_0^2}{b^4(t)} = 0. \tag{14}$$

It is simply that of weakly interacting bosons [43,44]. The evolution of contact is again determined by $\mathcal{C}(t) = \int d\mathbf{r}\mathcal{I}(\mathbf{r},t)$ with local contact density [15]

$$\mathcal{I}(\mathbf{r},t) \approx \frac{4\pi n(\mathbf{r},t)}{a} + \pi^2 n^2(\mathbf{r},t)a_m a, \tag{15}$$

where $a_m \approx 0.6a$ is the scattering length between molecules [45]. Then we have $\mathcal{C}(t) = \mathcal{C}_b + \mathcal{C}_m b^{-3}$, in which $\mathcal{C}_b = 4\pi N/a$ is the contribution from the binding energy of the tightly bound molecules that is not released during expansion. $\mathcal{C}_m = \int d\mathbf{r}\pi^2 n_0^2(\mathbf{r})a_m a$ is the initial contact corresponding to the interaction energy between molecules, i.e., $E_{m,\rm int}^{(0)} = \hbar^2\mathcal{C}_m/4\pi ma$. From the dynamic virial theorem, the release energy is easily calculated, i.e.,

$$\begin{aligned} E_{\rm rel} &\equiv E + \frac{N\epsilon_b}{2} \\ &= \left[\frac{1}{3b^3(t)} + \frac{2}{3}\right]E_{\rm ho}^{(0)} - \frac{1}{2b^3(t)}E_{m,\rm int}^{(0)}, \end{aligned} \tag{16}$$

where $\epsilon_b = \hbar^2/ma^2$ is the binding energy of molecules. By further using the equilibrium virial theorem for weakly interacting bosons initially in the trap, $E_{m,\rm int}^{(0)} = 2E_{\rm ho}^{(0)}/3$ [46], the release energy simply becomes $E_{\rm rel} = 2E_{\rm ho}^{(0)}/3$, the well-known result in the BEC limit [2].

In the unitarity limit with divergent scattering length, the release energy is rather easy to calculate since the system obeys an exact scale-invariant evolution, which yields $b(t) = \sqrt{1+\omega_0^2 t^2}$ [32,36]. In addition, the second term on the right-hand side of Eq. (1) vanishes in the unitarity limit. Consequently, the dynamic virial theorem simply gives the well-known result $E_{\rm rel} = E_{\rm ho}^{(0)}$ [2].

Another application of free expansion is to test the scale invariance of strongly interacting quantum gases as well as important consequences resulting from the scale-symmetry breaking [25,47,48]. Such scale-invariant dynamics could be identified according to the evolution of the cloud size, which is governed by the dynamic virial theorem. If defining

$$\tau^2(t) \equiv \frac{m}{2E_{\rm ho}^{(0)}}(\langle r^2\rangle - \langle r^2\rangle_0), \tag{17}$$

we easily obtain the equation satisfied by $\tau^2(t)$,

$$\frac{d^2}{dt^2}\tau^2(t) = 2 + \frac{\hbar^2[\mathcal{C}(t) - \mathcal{C}_0]}{4\pi maE_{\rm ho}^{(0)}}, \tag{18}$$

where $\mathcal{C}_0$ is the initial contact before release. In [25], $\tau^2(t)$, as an identification of the scale invariance, is measured in the free expansion and obeys $\tau^2(t) = t^2$ for a scale-invariant Fermi gas. In the weakly interacting limit, we obtain

$$\frac{d^2}{dt^2}\tau^2(t) \approx 2 + 0.29278k_{FI}a\left[\left(1+\omega_0^2 t^2\right)^{-3/2} - 1\right] \tag{19}$$

and

$$\frac{d^2}{dt^2}\tau^2(t) \approx 2 + 2.4668(k_{FI}a)^{-1}\left[\left(1+\omega_0^2 t^2\right)^{-1/2} - 1\right] \tag{20}$$

in the strongly interacting limit, where k_{FI} is the Fermi wave number at trap center for an ideal gas. Generally, an accurate estimation of contact is needed to depict the evolution of $\tau^2(t)$ in the free expansion, for example, by using high-temperature virial expansion [25,49,50].

IV. EFIMOVIAN EXPANSION

Scale-invariant quantum gases display a fancy scaling expansion dynamics in time-dependent harmonic traps, i.e., $\omega(t) \sim 1/\sqrt{\lambda}t$, with variation rate λ. This phenomenon is termed "Efimovian expansion" [26]. Here, we show that such profound expansion dynamics is inherently governed by the dynamic virial theorem. By further taking the derivative of dynamic virial theorem with respect to t, we obtain

$$\frac{1}{4}\frac{d^3I}{dt^3} = \frac{dE}{dt} - 2\frac{dE_{\rm ho}}{dt} + \frac{\hbar^2}{8\pi ma}\frac{d\mathcal{C}}{dt}. \tag{21}$$

According to the Hellmann-Feynman theorem, we have

$$\frac{dE}{dt} = \frac{d}{dt}\langle\hat{H}(t)\rangle = \left\langle\frac{d}{dt}\hat{H}(t)\right\rangle = -\frac{I(t)}{\lambda t^3}. \tag{22}$$

Combining with $E_{\rm ho} = I/2\lambda t^2$, we arrive at

$$\frac{d^3I}{dt^3} + \frac{4}{\lambda t^2}\frac{dI}{dt} - \frac{4I}{\lambda t^3} = \frac{\hbar^2}{2\pi ma}\frac{d\mathcal{C}}{dt}. \tag{23}$$

For noninteracting and resonant-interacting (scale-invariant) Fermi gases, the right-hand side of Eq. (23) vanishes, which recovers that of [26,51]. The evolution of cloud size demonstrates a temporal scaling expansion behavior. Away from the scale-invariant point at finite interaction strength, the expansion dynamics resulting from the scale-symmetry breaking is simply characterized by the evolution of contact [52–54]. In the strongly interacting limit, the contact can approximately be estimated as before, i.e., $\mathcal{C}(t) \approx \mathcal{C}_0/b(t)$ with $b^2(t) = I(t)/I_0$. Here, I_0 is the initial moment of inertia and $\mathcal{C}_0 = 256\pi\alpha N k_{FI}/35\xi_B^{1/4}$ is the initial contact [41,46], where N is the total atom number, and $\alpha \approx 0.12$ and $\xi_B \approx 0.37$ are universal parameters. The evolution of cloud size (or moment of inertia) during Efimovian expansion near resonant interaction is shown in Fig. 1.

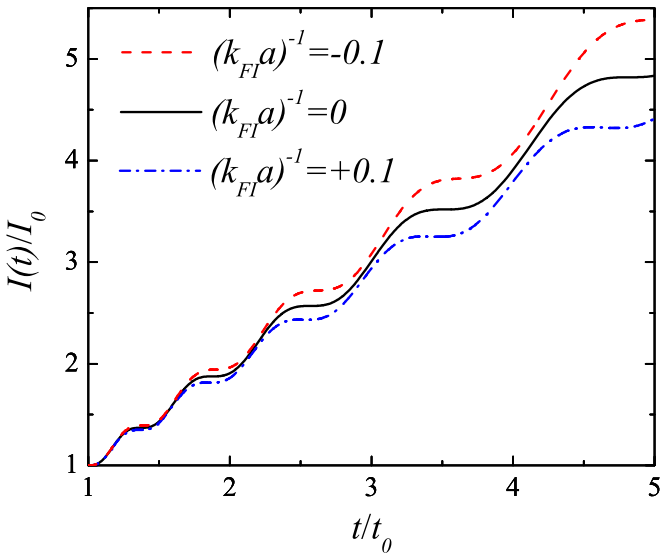

FIG. 1. Efimovian expansion of a two-component Fermi gas near resonance. Here, the variation rate of the trap is set to be $\lambda = 0.01$, t_0 is the initial time, I_0 is the initial moment of inertia (or cloud size), and k_{FI} is the initial Fermi wave number at the trap center for an ideal gas.

V. MONOPOLE OSCILLATIONS

The study of low-energy elementary excitations is a subject of primary importance in many-body physics. It is achieved, for example, by abruptly disturbing the external trap and exerting the oscillation of the system around its equilibrium. In the following, let us discuss the monopole oscillation of cold atoms in a spherical trap, which we find is governed by the dynamic virial theorem.

Let us first consider a cluster of classical particles in a harmonic trap interacting according to short-range potentials. The moment of inertia of a single particle is defined as $I \equiv mr^2$. Then we have $\dot{I} = 2\mathbf{p}\cdot\mathbf{r}$ with the momentum $\mathbf{p}$. By further taking the second-order derivative with respect to t, we obtain $\ddot{I} = 2(\dot{\mathbf{p}}\cdot\mathbf{r} + \mathbf{p}\cdot\dot{\mathbf{r}})$. As we have $\dot{\mathbf{p}} = \mathbf{F}$, the force acting on the particle, and the kinetic energy $E_{\rm kin} = \mathbf{p}\cdot\dot{\mathbf{r}}/2$, we obtain $\ddot{I} = 2(\mathbf{F}\cdot\mathbf{r} + 2E_{\rm kin})$. In the harmonic trap, the force acting on the particle is the negative gradient of the potential energy, i.e., $\mathbf{F} = -\nabla E_{\rm ho}$, which immediately gives $\mathbf{F}\cdot\mathbf{r} = -2E_{\rm ho}$. Finally, we obtain $E(t) - 2E_{\rm ho}(t) = \ddot{I}(t)/4$. Since the interactions between the atoms are local, the positions of the atoms as well as their moment of inertia are not changed from the instant before to the instant after collision. Therefore, the momentum and energy conversation implies that [27]

$$E(t) - 2E_{\rm ho}(t) = \frac{1}{4}\frac{d^2I}{dt^2} \tag{24}$$

holds for a cluster of classical particles. Equation (24) is the classical version of the dynamic virial theorem. The classical dynamic virial theorem simply leads to a nondamping monopole oscillation with the frequency $\omega_M = 2\omega_0$, which has recently been observed in a Bose gas [27].

In the low-temperature limit, quantum correlations resulting from interactions come into play. Let us consider the small monopole oscillation of a two-component Fermi gas initially prepared at equilibrium in the trap. Then the total energy of the system is given by the virial theorem, and we have $E = [2 - \chi(g)/2]E_{\rm ho}^{(0)}$ in the BCS limit, $E = 2E_{\rm ho}^{(0)}$ in the unitarity limit, and $E = 5E_{\rm ho}^{(0)}/3 - N\epsilon_b/2$ in the BEC limit. Here, $\chi(g) = E_{\rm int}^{(0)}/E_{\rm ho}^{(0)}$ is the ratio of the interaction energy $E_{\rm int}^{(0)}$ to the potential energy $E_{\rm ho}^{(0)}$, ϵ_b is the binding energy of molecules, and N is the atom number. At time $t = 0$, the monopole oscillation is exerted due to a slight disturbing on the trap. The evolution of contact is easily evaluated by using the adiabatic ansatz as before. Then the evolution of the moment of inertia or the cloud size is given by the dynamic virial theorem.

In the BCS limit, we obtain

$$\frac{d^2y}{dt^2} + 4\omega_0^2 y - \omega_0^2\chi(g)y^{-3/2} - 2\omega_0^2\left[2 - \frac{\chi(g)}{2}\right] = 0, \tag{25}$$

where we have defined $y \equiv \langle r^2\rangle(t)/\langle r^2\rangle(0)$. By linearizing Eq. (25) around the equilibrium, i.e., $y \approx 1 + \delta y$, we obtain

$$\frac{d^2\delta y}{dt^2} + \left[4 + \frac{3}{2}\chi(g)\right]\omega_0^2\delta y = 0. \tag{26}$$

We find that the frequency of the monopole oscillation is shifted to $\omega_M = \omega_0\sqrt{4+3\chi(g)/2}$ by interatomic interactions. It further reduces to $\omega_M = 2\omega_0$ in the noninteracting limit. In the BEC limit, we similarly have

$$\frac{d^2y}{dt^2} + 4\omega_0^2 y - \frac{2}{3}\omega_0^2 y^{-3/2} - \frac{10}{3}\omega_0^2 = 0, \tag{27}$$

which is linearized to

$$\frac{d^2\delta y}{dt^2} + 5\omega_0^2\delta y = 0. \tag{28}$$

The frequency of the monopole oscillation is then shifted to $\omega_M = \sqrt{5}\omega_0$ in the BEC limit, consistent with the well-known result of Bose gases in the presence of mean-field interactions. In the unitarity limit, the dynamic virial theorem implies that a strongly interacting Fermi gas exactly follows the same monopole oscillation as that of an ideal gas with the frequency $\omega_M = 2\omega_0$.

VI. MAXIMUM ENERGY GROWTH UNDER INCREASING INTERACTIONS

In this section, let us discuss the dynamic behavior of interacting many-body systems with time-dependent interatomic interactions. Explicitly, we consider how fast the energy could be pumped into a system by increasing interactions, starting from the noninteracting limit. This fundamental issue has recently been addressed [34]. Counterintuitively, it is not true that the faster the interaction increases, the larger the rate of energy gain becomes. The maximum energy growth theorem states that there exists an upper limit of initial energy growth rate, which could be reached only when the scattering length increases with time t as $\sim\sqrt{t}$. However, the direct measurement of the energy dynamics in experiments is difficult. Here, we are going to show that the dynamic virial theorem provides an experimentally accessible way to verify the maximum energy growth theorem according to the evolution of the cloud size during expansion.

Let us consider a two-component Fermi gas initially prepared at equilibrium in the trap. It is supposed that the initial interatomic interaction is so weak that we may treat it as an ideal gas. Then the gas is released from the trap for $t \geqslant 0$, accompanied by the increase of interactions. To estimate the *initial* energy growth rate, it is sufficient to consider the dynamics of the system in short time. Here, the short time is defined as the timescale much smaller than the many-body timescale $t_n = \hbar/E_F$ related to the Fermi energy E_F, and also larger than the timescale $t_r = mr_0^2/\hbar$ imposed by the range r_0 of the two-body potential. In this timescale, the scattering length may be assumed to take a power-law form of

$$a(t) = a_{\rm ho}\beta(\omega_0 t)^\alpha, \tag{29}$$

and the two-body physics dominates the expansion dynamics. Here, $a_{\rm ho} = \sqrt{\hbar/m\omega_0}$ is the harmonic length with respect to the initial trap with frequency ω_0, and α, $\beta > 0$ are parameters that characterize, respectively, the power and quench rate. Then the energy can be obtained by simply integrating Tan's sweep theorem over time t, i.e.,

$$E(t) = E(0) + \int_0^t dt' \frac{\hbar^2\mathcal{C}(t')}{4\pi m a^2(t')}\frac{da}{dt'}, \tag{30}$$

where $E(0)$ is the initial energy that is simply the potential energy $E_{\rm ho}(0)$ given by the virial theorem at equilibrium. The evolution of the cloud size or the moment of inertia is related to the energy characterized by the dynamic virial theorem in expansion,

$$\frac{d^2I}{dt^2} = 4E(t) + \frac{\hbar^2\mathcal{C}(t)}{2\pi m a(t)}. \tag{31}$$

Inserting Eq. (30) into (31), we obtain

$$\frac{d^2I}{dt^2} = 2\omega_0^2 I_0 + \frac{\hbar^2\mathcal{C}(t)}{2\pi m a(t)} + \frac{\hbar^2}{\pi m}\int_0^t dt' \frac{\mathcal{C}(t')}{a^2(t')}\frac{da}{dt'}, \tag{32}$$

and $I_0 = 2E_{\rm ho}(0)/\omega_0^2$ is the initial moment of inertia. We find that the dynamics of Tan's contact is crucial for evaluating the energy as well as the cloud size, which is simply governed by the two-body physics in short time as pointed out in [34]. There are totally three typical behaviors of the evolution of contact in short time, depending on the power parameter α [34], i.e.,

$$\mathcal{C}(t) = \begin{cases} 16\pi^2 g_2(0)a^2(t), & \alpha > 1/2 \\ |A(\beta)|^2 g_2(0)\hbar t/m, & \alpha = 1/2 \\ |A(\infty)|^2 g_2(0)\hbar t/m, & 0 < t < 1/2, \end{cases} \tag{33}$$

where $g_2(\mathbf{r})$ is defined as

$$g_2(\mathbf{r}) \equiv \int d\mathbf{R}\rho_2(\mathbf{R}+\mathbf{r}/2, \mathbf{R}-\mathbf{r}/2), \tag{34}$$

and

$$\rho_2(\mathbf{r}_1, \mathbf{r}_2) = \langle\hat{\psi}_\uparrow^\dagger(\mathbf{r}_1)\hat{\psi}_\downarrow^\dagger(\mathbf{r}_2)\hat{\psi}_\downarrow(\mathbf{r}_2)\hat{\psi}_\uparrow(\mathbf{r}_1)\rangle_0 \tag{35}$$

is the two-body density matrix for the initial state. Here, it is defined $A(\beta) = [B(1/2) + 1/4\pi\beta]^{-1}$ and $B(\alpha) = i^{3/2}\Gamma(\alpha+1)/4\pi\Gamma(\alpha+1/2)$. Subsequently, the energy as well as the evolution of the moment of inertia can conveniently be evaluated as follows.

For $\alpha > 1/2$, the contact takes the form of

$$\mathcal{C}(t) = 16\pi^2 g_2(0)a^2(t) = 16\pi^2 g_2(0)a_{\rm ho}^2\beta^2(\omega_0 t)^{2\alpha}. \tag{36}$$

The energy growth $\delta E(t) \equiv E(t) - E(0)$ in short time is obtained according to Eq. (30),

$$\frac{\delta E(t)}{g_2(0)a_{\rm ho}^3\hbar\omega_0} = 4\pi\beta(\omega_0 t)^\alpha. \tag{37}$$

By inserting Eqs. (29) and (36) into Eq. (32), the evolution of the moment of inertia in short time satisfies

$$\frac{d^2I}{dt^2} = 2\omega_0^2 I_0 + \frac{24\pi\hbar^2\beta}{m}g_2(0)a_{\rm ho}(\omega_0 t)^\alpha. \tag{38}$$

Combining with the initial conditions $I(0)/I_0 = 1$ and $\dot{I}(0)/I_0 = 0$, we obtain

$$f_0^{-1}\left[\frac{I}{I_0} - (1+(\omega_0 t)^2)\right] = \frac{12\pi\beta}{(1+\alpha)(2+\alpha)}(\omega_0 t)^{2+\alpha}, \tag{39}$$

with $f_0 = g_2(0)a_{\rm ho}^3\hbar\omega_0/E_{\rm ho}(0)$. If defining the reduced moment of inertia and energy growth as

$$\tilde{I}(t) \equiv f_0^{-1}\left[\frac{I}{I_0} - (1+(\omega_0 t)^2)\right], \tag{40}$$

$$\delta\tilde{E}(t) \equiv \frac{\delta E(t)}{\hbar\omega_0 g_2(0)a_{\rm ho}^3}, \tag{41}$$

we easily find a one-on-one correspondence between the energy growth and the moment of inertia,

$$\delta\tilde{E}(t) = 4\pi\beta\left[\frac{(1+\alpha)(2+\alpha)}{12\pi\beta}\tilde{I}(t)\right]^{\alpha/(2+\alpha)}. \quad (42)$$

At the critical point of $\alpha = 1/2$, we have

$$a(t) = \beta a_{\rm ho}(\omega_0 t)^{1/2} = \beta\left(\frac{\hbar}{m}\right)^{1/2} t^{1/2}, \quad (43)$$

and the contact is linearly dependent on time, i.e., $\mathcal{C}(t) = |A(\beta)|^2 g_2(0)\hbar t/m$. Then the reduced initial energy growth takes the form of

$$\delta\tilde{E}(t) = \frac{|A(\beta)|^2(\omega_0 t)^{1/2}}{4\pi\beta}. \quad (44)$$

Similarly, according to the dynamic virial theorem, the evolution of the moment of inertia satisfies

$$\frac{d^2 I}{dt^2} = 2\omega_0^2 I_0 + \frac{3\hbar^2}{2\pi m\beta}|A(\beta)|^2 g_2(0) a_{\rm ho}(\omega_0 t)^{1/2}, \quad (45)$$

which yields

$$\tilde{I}(t) = \frac{|A(\beta)|^2(\omega_0 t)^{5/2}}{5\pi\beta}. \quad (46)$$

Then we arrive at the one-on-one correspondence between the reduced initial energy growth and the moment of inertia,

$$\delta\tilde{E}(t) = \frac{|A(\beta)|^{8/5}}{4\pi\beta}[5\pi\beta\tilde{I}(t)]^{1/5}. \quad (47)$$

For $0 < \alpha < 1/2$, the evolution of the contact linearly increases with time as well, i.e., $\mathcal{C}(t) = |A(\infty)|^2 g_2(0)\hbar t/m$, and is independent of the parameters α and β. This means that the contact is independent of how fast the scattering length varies in time, even if the scattering length initially grows infinitely fast as in the quench process. In this case, the corresponding reduced energy growth becomes

$$\delta\tilde{E}(t) = \frac{16\alpha}{\beta(1-\alpha)}(\omega_0 t)^{1-\alpha}. \quad (48)$$

Again the evolution of the moment of inertia is given by the dynamic virial theorem,

$$\frac{d^2 I}{dt^2} = 2\omega_0^2 I_0 + \frac{32\hbar^2 a_{\rm ho}}{m\beta}\frac{1+\alpha}{1-\alpha}g_2(0)(\omega_0 t)^{1-\alpha}, \quad (49)$$

which yields

$$\tilde{I}(t) = \frac{16(1+\alpha)}{\beta(1-\alpha)(2-\alpha)(3-\alpha)}(\omega_0 t)^{3-\alpha}. \quad (50)$$

Then we arrive at the relation

$$\delta\tilde{E}(t) = \frac{16\alpha}{\beta(1-\alpha)} \times \left[\frac{\beta(1-\alpha)(2-\alpha)(3-\alpha)}{16(1+\alpha)}\tilde{I}(t)\right]^{(1-\alpha)/(3-\alpha)}. \quad (51)$$

Until now, we have obtained the one-on-one correspondence between the instantaneous energy gain and the moment of inertia (or cloud size). The initial energy growth as a function of the atomic cloud size is plotted in Fig. 2 for several typical power parameters. The energy gain resulting from the interaction increasing can conveniently be measured in experiments according to the measurement of the cloud size in expansion. We find that expanding to the same size, the energy gain of the system reaches the maximum when the scattering length increases as $\sim\sqrt{t}$, which provides an identification of the maximum energy growth theorem in experiments.

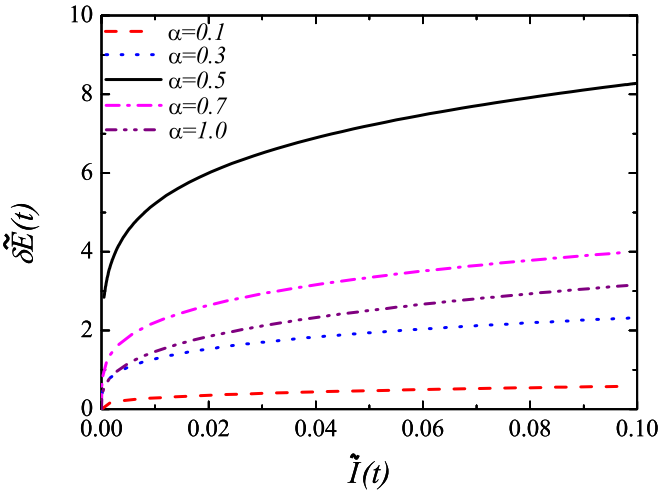

FIG. 2. The initial energy growth as a function of the atomic cloud size during the expansion accompanied by an increasing of the scattering length $a(t)/a_{\rm ho} = \beta(\omega_0 t)^\alpha$ at different power parameters. Here, we set $\beta = 1$.

VII. THERMODYNAMIC RELATION

In the following, we derive an out-of-equilibrium thermodynamic relation for interacting quantum gases. Here, a two-fluid hydrodynamic theory is adopted to study the dynamics at nonequilibrium, which is applicable in a wide range of temperatures. The basic idea of the two-fluid hydrodynamic theory lies in considering the system as if it were a mixture of two different liquids at finite temperature: A superfluid without viscosity and a viscous normal fluid. Analogous to those for superfluids or normal fluids, the number density of particles satisfies the equation of continuity,

$$\frac{\partial n}{\partial t} + \nabla\cdot\mathbf{j} = 0, \quad (52)$$

where $n = n_n + n_s$ is the total number density, and $\mathbf{j} = n_n\mathbf{v}_n + n_s\mathbf{v}_s$ is the current density with the number density $n_{s(n)}$ for the superfluid (normal) component and the corresponding velocity $\mathbf{v}_{s(n)}$. In addition, the current density $\mathbf{j}$ satisfies an additional equation [55],

$$\frac{\partial j_i}{\partial t} + \sum_k \frac{\partial \Pi_{ik}}{\partial x_k} + \frac{n}{m}\frac{\partial V_{\rm ext}}{\partial x_i} = -\sum_k \frac{\partial \Pi'_{ik}}{\partial x_k}, \quad (53)$$

for the ith component of $\mathbf{j}$, where $V_{\rm ext}$ is the external potential, Π_{ik} is the momentum current density tensor defined as

$$\Pi_{ik} \equiv n_n v_{ni} v_{nk} + n_s v_{si} v_{sk} + \frac{p}{m}\delta_{ik}, \quad (54)$$

and p is the pressure. The viscous normal fluid introduces an additional dissipation described by

$$\Pi'_{ik} = -\frac{\eta}{m}\sigma_{ik} - \delta_{ik}\left(\frac{\zeta_1}{m}\sigma'_1 + \frac{\zeta_2}{m}\sigma'_2\right), \tag{55}$$

with

$$\sigma_{ik} \equiv \frac{\partial v_{ni}}{\partial x_k} + \frac{\partial v_{nk}}{\partial x_i} - \frac{2}{3}\delta_{ik}\nabla\cdot\mathbf{v}_n, \tag{56}$$

$$\sigma'_1 \equiv \nabla\cdot[mn_s(\mathbf{v}_n - \mathbf{v}_s)], \tag{57}$$

$$\sigma'_2 \equiv \nabla\cdot\mathbf{v}_n. \tag{58}$$

Here, η and $\zeta_{1,2}$ are, respectively, the shear and bulk viscosities. Equations (52) and (53) forms a set of basic equations to describe the dynamics of interacting quantum gases at finite temperature.

At zero temperature, the system becomes a pure superfluid, and the number density of the normal component vanishes as well as corresponding velocities. Then, Eq. (53) becomes

$$\frac{\partial(nv_i)}{\partial t} + \sum_k \frac{\partial}{\partial x_k}(nv_iv_k) + \frac{1}{m}\frac{\partial p}{\partial x_i} + \frac{n}{m}\frac{\partial V_{\rm ext}}{\partial x_i} = 0, \tag{59}$$

which, combined with the equation of continuity, yields

$$\frac{\partial\mathbf{v}}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{v} + \frac{\nabla p}{mn} + \frac{\nabla V_{\rm ext}}{m} = 0. \tag{60}$$

By using the identity of

$$\nabla\left(\frac{v^2}{2}\right) = \mathbf{v}\times(\nabla\times\mathbf{v}) + (\mathbf{v}\cdot\nabla)\mathbf{v}, \tag{61}$$

and concerning the fact that the superfluid corresponds to a potential flow with $\nabla\times\mathbf{v} = 0$, we arrive at

$$\frac{\partial\mathbf{v}}{\partial t} + \nabla\left(\frac{v^2}{2}\right) + \frac{\nabla p}{mn} + \frac{\nabla V_{\rm ext}}{m} = 0. \tag{62}$$

This is the well-known Euler equation for a superfluid (see, for example, [56]). Here, all the quantities are those for the superfluid so that the subscript s is dropped off without confusion.

Above the critical temperature, the system is entirely a normal fluid and the superfluid portion vanishes. Then, Eq. (53) becomes the Euler equation for a normal fluid in the presence of viscosity at finite temperature [25,55], i.e.,

$$\left[nm\frac{\partial}{\partial t} + nm(\mathbf{v}\cdot\nabla)\right]v_i + \frac{\partial p}{\partial x_i} + n\frac{\partial V_{\rm ext}}{\partial x_i} = \sum_k \frac{\partial}{\partial x_k}(\eta\sigma_{ik} + \delta_{ik}\zeta_2\sigma'_2). \tag{63}$$

Consequently, we find that the two-fluid hydrodynamic theory provides a rather general formulism to describe the dynamics of interacting many-body systems in a wide range of temperatures. Moreover, the quantum pressure comes into play at zero temperature, which could formally be included in the definition of pressure, i.e., $p = p_c + p_q$ and $p_{c(q)}$ stands for the classical (quantum) pressure [57].

Now we are ready for the discussion of the evolution of moment of inertia $I(t) \equiv \langle mr^2\rangle$ based on the two-fluid hydrodynamic formulism. The ith component of $\langle r^2\rangle$ is defined as $\langle x_i^2\rangle = \int d\mathbf{r} n x_i^2$, with $i = x, y, z$, which obeys

$$\frac{d\langle x_i^2\rangle}{dt} = \int d\mathbf{r}\frac{\partial n}{\partial t}x_i^2 = -\int d\mathbf{r}(\nabla\cdot\mathbf{j})x_i^2 = 2\int d\mathbf{r}\, j_i x_i. \tag{64}$$

By further taking the second-order derivative with respect to t, we have

$$\frac{d^2\langle x_i^2\rangle}{dt^2} = 2\int d\mathbf{r}\frac{\partial j_i}{\partial t}x_i. \tag{65}$$

According to Eq. (53), we obtain

$$\frac{d^2\langle x_i^2\rangle}{dt^2} = 2\int d\mathbf{r}(\Pi_{ii} + \Pi'_{ii}) - 2\int d\mathbf{r}x_i\frac{n}{m}\frac{\partial V_{\rm ext}}{\partial x_i}. \tag{66}$$

By inserting the explicit form of $\Pi_{ii}^{(\prime)}$ into the above equation and assuming that the external potential is a harmonic trap, i.e., $V_{\rm ext}(\mathbf{r}) = m\omega^2 r^2/2$, we arrive at

$$\frac{1}{4}\frac{d^2\langle x_i^2\rangle}{dt^2} = \int d\mathbf{r}\left[n_n\frac{v_{ni}^2}{2} + n_s\frac{v_{si}^2}{2} + \frac{p}{2m} - \frac{\eta}{2m}\sigma_{ii} - \frac{1}{2m}(\zeta_1\sigma'_1 + \zeta_2\sigma'_2)\right] - \int d\mathbf{r}\frac{n}{m}\left(\frac{1}{2}m\omega^2 x_i^2\right). \tag{67}$$

Summing the above equation over all three directions and noticing $\sum_i\int d\mathbf{r}\eta\sigma_{ii} = 0$, we finally obtain

$$\frac{1}{4}\frac{d^2I}{dt^2} = E_{\rm kin} - E_{\rm ho} + \frac{3}{2}\mathcal{J} - \frac{3}{2}\int d\mathbf{r}(\zeta_1\sigma'_1 + \zeta_2\sigma'_2), \tag{68}$$

where $E_{\rm kin} \equiv \int d\mathbf{r}(n_n mv_n^2 + n_s mv_s^2)/2$ corresponds to the total kinetic energy of the normal fluid and superfluid, $E_{\rm ho} = \int d\mathbf{r}n(m\omega^2r^2/2)$ is the potential energy, and $\mathcal{J} \equiv \int d\mathbf{r}p$ is the integral of the local pressure over the whole space, namely, the thermodynamic potential. Equation (68) simply reduces to that for a normal fluid with $\zeta_1 = 0$ above the critical temperature [25].

Combining Eq. (68) and the dynamic virial theorem, we find the following simple relation for interacting quantum gases:

$$\mathcal{J} = \frac{2}{3}E_{\rm internal}(t) + \frac{\hbar^2\mathcal{C}(t)}{12\pi ma(t)} + \Gamma(t), \tag{69}$$

where we have defined the internal energy $E_{\rm internal} \equiv E(t) - E_{\rm kin}(t) - E_{\rm ho}(t)$ and the dissipation energy resulting from viscosities, $\Gamma(t) = \int d\mathbf{r}(\zeta_1\sigma'_1 + \zeta_2\sigma'_2)$. This relation holds for both the normal fluid and superfluid as well as their mixtures, and thus is valid in a wide range of temperatures. Equation (69) is a kind of the out-of-equilibrium analog of Tan's pressure relation since it simply reduces to the well-known form for uniform gases at equilibrium [16], i.e.,

$$p = \frac{2}{3}\mathcal{E}_{\rm internal} + \frac{\hbar^2\mathcal{I}}{12\pi ma}, \tag{70}$$

with the internal energy density $\mathcal{E}_{\rm internal}$, the contact density $\mathcal{I} = \mathcal{C}/V$, and the volume V.

VIII. CONCLUSIONS

It is shown that a variety of out-of-equilibrium dynamics of interacting many-body systems is elegantly governed by the dynamic virial theorem. Its applications in several typical nonequilibrium dynamic processes of cold atoms are presented, in which observable consequences in experiments are discussed. Remarkably, the dynamic virial theorem provides an experimentally accessible way to verify the maximum energy growth theorem according to the measurement of the atomic cloud size in expansion. In addition, the dynamic virial theorem gives rise to a simple thermodynamic relation, the analog of Tan's pressure relation at equilibrium, for interacting many-body systems in the framework of two-fluid hydrodynamic theory. This thermodynamic relation holds in a wide range of temperatures. Our results provide a fundamental understanding of the generic behaviors of interacting many-body systems at nonequilibrium and are readily examined in future experiments with ultracold atoms.

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